



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 31, 2023 – 07:33 PM JST

PDB ID : 5GWK
Title : Human topoisomerase IIalpha in complex with DNA and etoposide
Authors : Wang, Y.R.; Wu, C.C.; Chan, N.L.
Deposited on : 2016-09-12
Resolution : 3.15 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

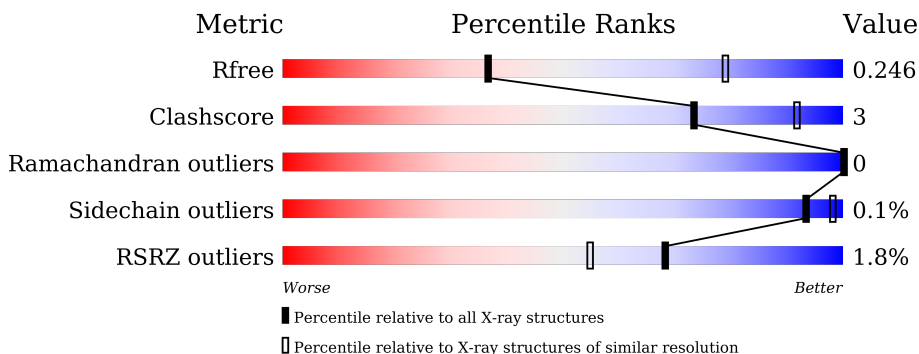
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (3.20-3.12)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	806	 0% 82% 8% 10%
1	B	806	 2% 81% 8% 10%
2	C	8	 100%
2	E	8	 12% 88% 12%
3	D	12	 8% 58% 42%
3	F	12	 67% 33%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	MG	B	1302	-	-	-	X

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 12670 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA topoisomerase 2-alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	724	5880	3756	999	1099	26	0	0	0
1	B	724	5880	3756	999	1099	26	0	0	0

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	403	MET	-	expression tag	UNP P11388
A	404	ALA	-	expression tag	UNP P11388
A	405	SER	-	expression tag	UNP P11388
A	406	TRP	-	expression tag	UNP P11388
A	407	SER	-	expression tag	UNP P11388
A	408	HIS	-	expression tag	UNP P11388
A	409	PRO	-	expression tag	UNP P11388
A	410	GLN	-	expression tag	UNP P11388
A	411	PHE	-	expression tag	UNP P11388
A	412	GLU	-	expression tag	UNP P11388
A	413	LYS	-	expression tag	UNP P11388
A	414	GLY	-	expression tag	UNP P11388
A	415	ALA	-	expression tag	UNP P11388
A	416	ASP	-	expression tag	UNP P11388
A	417	ASP	-	expression tag	UNP P11388
A	418	ASP	-	expression tag	UNP P11388
A	419	ASP	-	expression tag	UNP P11388
A	420	LYS	-	expression tag	UNP P11388
A	421	VAL	-	expression tag	UNP P11388
A	422	PRO	-	expression tag	UNP P11388
A	423	ASP	-	expression tag	UNP P11388
A	424	PRO	-	expression tag	UNP P11388
A	425	THR	-	expression tag	UNP P11388
A	426	SER	-	expression tag	UNP P11388
A	427	VAL	-	expression tag	UNP P11388

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Chain	Residue	Modelled	Actual	Comment	Reference
A	428	ASP	-	expression tag	UNP P11388
A	1189	GLY	-	expression tag	UNP P11388
A	1190	ALA	-	expression tag	UNP P11388
A	1191	PRO	-	expression tag	UNP P11388
A	1192	GLY	-	expression tag	UNP P11388
A	1193	PHE	-	expression tag	UNP P11388
A	1194	SER	-	expression tag	UNP P11388
A	1195	SER	-	expression tag	UNP P11388
A	1196	ILE	-	expression tag	UNP P11388
A	1197	SER	-	expression tag	UNP P11388
A	1198	ALA	-	expression tag	UNP P11388
A	1199	HIS	-	expression tag	UNP P11388
A	1200	HIS	-	expression tag	UNP P11388
A	1201	HIS	-	expression tag	UNP P11388
A	1202	HIS	-	expression tag	UNP P11388
A	1203	HIS	-	expression tag	UNP P11388
A	1204	HIS	-	expression tag	UNP P11388
A	1205	HIS	-	expression tag	UNP P11388
A	1206	HIS	-	expression tag	UNP P11388
A	1207	HIS	-	expression tag	UNP P11388
A	1208	HIS	-	expression tag	UNP P11388
B	403	MET	-	expression tag	UNP P11388
B	404	ALA	-	expression tag	UNP P11388
B	405	SER	-	expression tag	UNP P11388
B	406	TRP	-	expression tag	UNP P11388
B	407	SER	-	expression tag	UNP P11388
B	408	HIS	-	expression tag	UNP P11388
B	409	PRO	-	expression tag	UNP P11388
B	410	GLN	-	expression tag	UNP P11388
B	411	PHE	-	expression tag	UNP P11388
B	412	GLU	-	expression tag	UNP P11388
B	413	LYS	-	expression tag	UNP P11388
B	414	GLY	-	expression tag	UNP P11388
B	415	ALA	-	expression tag	UNP P11388
B	416	ASP	-	expression tag	UNP P11388
B	417	ASP	-	expression tag	UNP P11388
B	418	ASP	-	expression tag	UNP P11388
B	419	ASP	-	expression tag	UNP P11388
B	420	LYS	-	expression tag	UNP P11388
B	421	VAL	-	expression tag	UNP P11388
B	422	PRO	-	expression tag	UNP P11388
B	423	ASP	-	expression tag	UNP P11388

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Chain	Residue	Modelled	Actual	Comment	Reference
B	424	PRO	-	expression tag	UNP P11388
B	425	THR	-	expression tag	UNP P11388
B	426	SER	-	expression tag	UNP P11388
B	427	VAL	-	expression tag	UNP P11388
B	428	ASP	-	expression tag	UNP P11388
B	1189	GLY	-	expression tag	UNP P11388
B	1190	ALA	-	expression tag	UNP P11388
B	1191	PRO	-	expression tag	UNP P11388
B	1192	GLY	-	expression tag	UNP P11388
B	1193	PHE	-	expression tag	UNP P11388
B	1194	SER	-	expression tag	UNP P11388
B	1195	SER	-	expression tag	UNP P11388
B	1196	ILE	-	expression tag	UNP P11388
B	1197	SER	-	expression tag	UNP P11388
B	1198	ALA	-	expression tag	UNP P11388
B	1199	HIS	-	expression tag	UNP P11388
B	1200	HIS	-	expression tag	UNP P11388
B	1201	HIS	-	expression tag	UNP P11388
B	1202	HIS	-	expression tag	UNP P11388
B	1203	HIS	-	expression tag	UNP P11388
B	1204	HIS	-	expression tag	UNP P11388
B	1205	HIS	-	expression tag	UNP P11388
B	1206	HIS	-	expression tag	UNP P11388
B	1207	HIS	-	expression tag	UNP P11388
B	1208	HIS	-	expression tag	UNP P11388

- Molecule 2 is a DNA chain called DNA (5'-D(P*AP*GP*CP*CP*GP*AP*GP*C)-3').

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
2	C	8	Total	C	N	O	P	0	0	0
			165	77	34	46	8			
2	E	8	Total	C	N	O	P	0	0	0
			165	77	34	46	8			

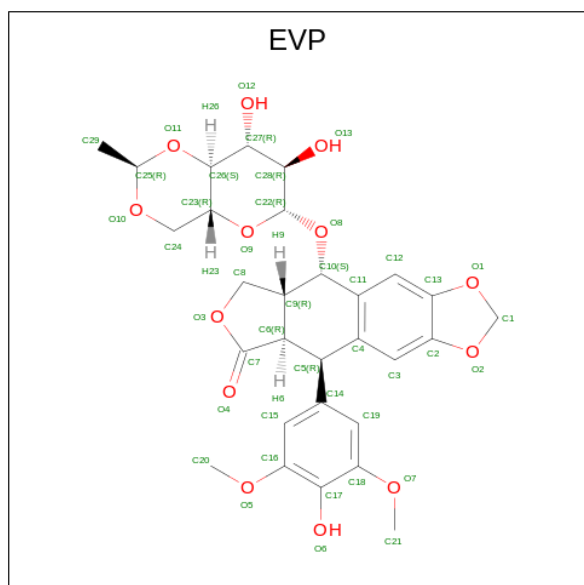
- Molecule 3 is a DNA chain called DNA (5'-D(P*TP*GP*CP*AP*GP*CP*TP*CP*GP*GP*CP*T)-3').

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
3	D	12	Total	C	N	O	P	0	0	0
			245	116	43	74	12			
3	F	12	Total	C	N	O	P	0	0	0
			245	116	43	74	12			

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Mg 2 2	0	0
4	B	2	Total Mg 2 2	0	0
4	D	1	Total Mg 1 1	0	0
4	F	1	Total Mg 1 1	0	0

- Molecule 5 is (5S,5aR,8aR,9R)-9-(4-hydroxy-3,5-dimethoxyphenyl)-8-oxo-5,5a,6,8,8a,9-hexahydrofuro[3',4':6,7]naphtho[2,3-d][1,3]dioxol -5-yl 4,6-O-[(1R)-ethylidene]-beta-D-glucopyranoside (three-letter code: EVP) (formula: C₂₉H₃₂O₁₃).

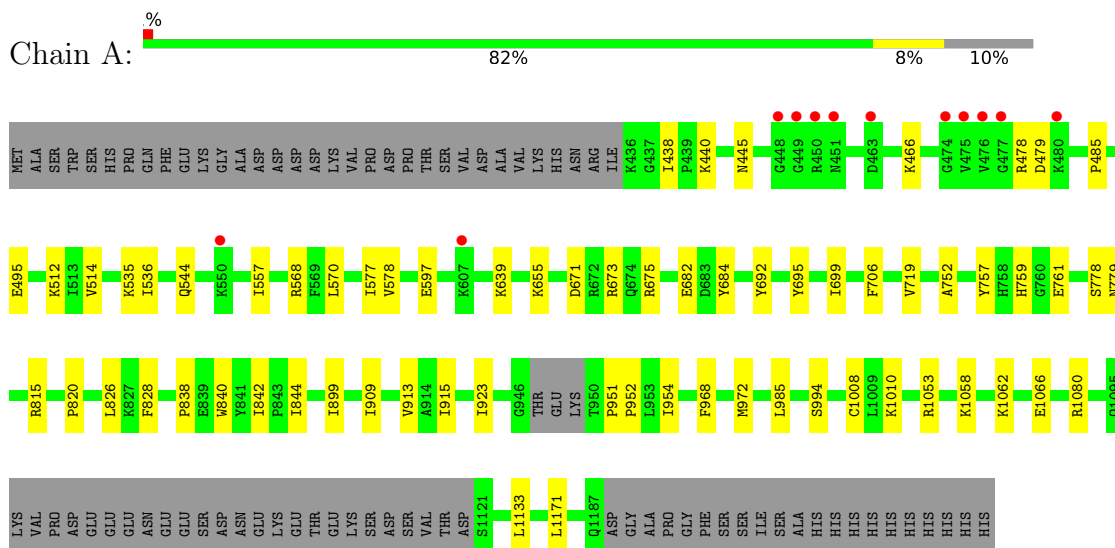


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total C O 42 29 13	0	0
5	F	1	Total C O 42 29 13	0	0

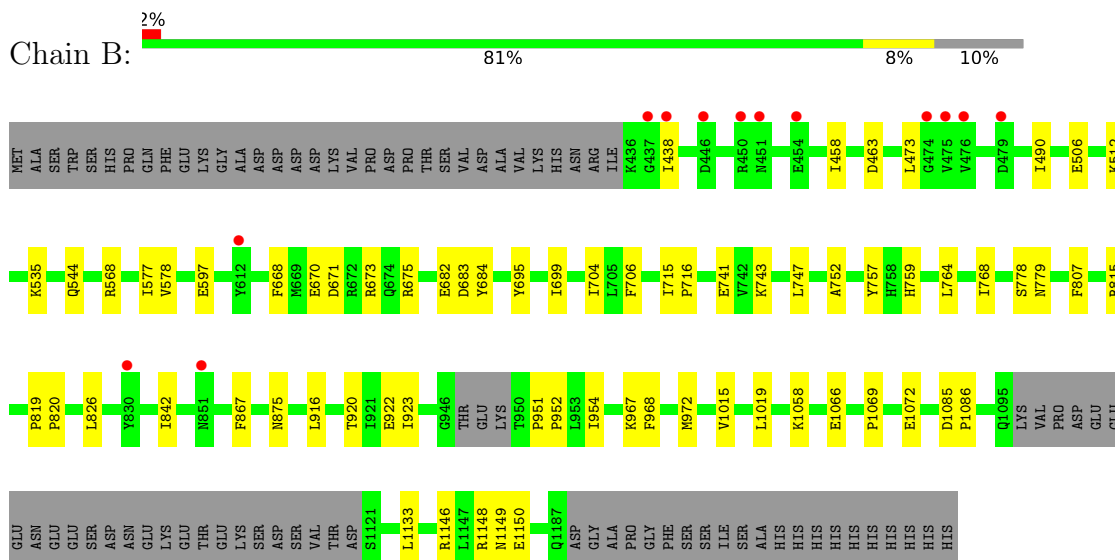
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: DNA topoisomerase 2-alpha



- Molecule 1: DNA topoisomerase 2-alpha




- Molecule 2: DNA (5'-D(P*AP*GP*CP*CP*GP*AP*GP*C)-3')

Chain C:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: DNA (5'-D(P*AP*GP*CP*CP*GP*AP*GP*C)-3')

Chain E:  12% 88% 12%



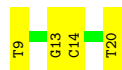
- Molecule 3: DNA (5'-D(P*TP*GP*CP*AP*GP*CP*TP*CP*GP*GP*CP*T)-3')

Chain D:  8% 58% 42%



- Molecule 3: DNA (5'-D(P*TP*GP*CP*AP*GP*CP*TP*CP*GP*GP*CP*T)-3')

Chain F:  67% 33%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 2 21	Depositor
Cell constants a, b, c, α , β , γ	105.11Å 126.16Å 198.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.49 – 3.15 27.49 – 3.15	Depositor EDS
% Data completeness (in resolution range)	99.1 (27.49-3.15) 96.1 (27.49-3.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.48	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.98 (at 3.17Å)	Xtrriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.203 , 0.244 0.206 , 0.246	Depositor DCC
R_{free} test set	2000 reflections (4.36%)	wwPDB-VP
Wilson B-factor (Å ²)	89.1	Xtrriage
Anisotropy	0.574	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 59.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12670	wwPDB-VP
Average B, all atoms (Å ²)	108.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.18% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, EVP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.21	0/6001	0.36	0/8088
1	B	0.21	0/6001	0.35	0/8088
2	C	0.52	0/185	0.75	0/283
2	E	0.50	0/185	0.73	0/283
3	D	0.54	0/273	0.93	0/419
3	F	0.56	0/273	0.94	0/419
All	All	0.25	0/12918	0.42	0/17580

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5880	0	5929	39	0
1	B	5880	0	5929	42	0
2	C	165	0	89	0	0
2	E	165	0	89	1	0
3	D	245	0	136	4	0
3	F	245	0	136	3	0
4	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	2	0	0	0	0
4	D	1	0	0	0	0
4	F	1	0	0	0	0
5	D	42	0	29	2	0
5	F	42	0	29	1	0
All	All	12670	0	12366	82	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (82) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:671:ASP:OD2	1:A:675:ARG:NH1	2.24	0.70
1:A:478:ARG:HG2	1:A:479:ASP:H	1.58	0.68
1:B:577:ILE:HG23	1:B:578:VAL:HG23	1.79	0.64
1:A:577:ILE:HG23	1:A:578:VAL:HG23	1.79	0.63
1:A:954:ILE:HA	1:A:972:MET:HG2	1.82	0.62
1:A:1062:LYS:HB3	1:A:1080:ARG:HH12	1.63	0.62
1:A:445:ASN:ND2	1:A:479:ASP:OD1	2.31	0.62
1:B:954:ILE:HA	1:B:972:MET:HG2	1.81	0.61
1:B:671:ASP:OD2	1:B:675:ARG:NH1	2.35	0.60
1:B:1146:ARG:NH1	1:B:1150:GLU:OE2	2.35	0.60
1:B:1148:ARG:NH1	1:B:1149:ASN:OD1	2.35	0.59
1:A:826:LEU:HD21	1:A:842:ILE:HG22	1.85	0.58
1:B:923:ILE:HB	1:B:968:PHE:HB2	1.86	0.58
3:D:9:DT:C2	5:F:102:EVP:H9	2.38	0.57
1:B:752:ALA:HA	1:B:757:TYR:HB3	1.88	0.56
1:B:826:LEU:HD21	1:B:842:ILE:HG22	1.87	0.55
1:A:828:PHE:HA	1:A:838:PRO:HA	1.89	0.55
1:B:535:LYS:NZ	1:B:568:ARG:O	2.39	0.55
1:A:923:ILE:HB	1:A:968:PHE:HB2	1.88	0.55
1:A:1058:LYS:NZ	1:B:1066:GLU:OE2	2.40	0.55
1:B:544:GLN:HB3	1:B:706:PHE:HA	1.89	0.55
1:B:922:GLU:OE2	1:B:967:LYS:NZ	2.40	0.54
1:A:673:ARG:NH1	1:A:1008:CYS:SG	2.81	0.54
1:A:761:GLU:OE2	1:B:743:LYS:NZ	2.39	0.54
1:A:752:ALA:HA	1:A:757:TYR:HB3	1.90	0.53
1:A:440:LYS:NZ	3:D:11:DC:OP1	2.41	0.53
1:A:1053:ARG:NH2	1:A:1080:ARG:O	2.34	0.53
1:B:463:ASP:OD1	5:D:102:EVP:O6	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1066:GLU:OE2	1:B:1058:LYS:NZ	2.43	0.52
1:A:1133:LEU:HD23	1:B:1133:LEU:HD23	1.90	0.52
1:B:438:ILE:HD11	1:B:512:LYS:HD3	1.92	0.51
3:D:20:DT:H3	2:E:1:DA:H2	1.60	0.50
1:A:757:TYR:CZ	1:A:759:HIS:HB2	2.47	0.50
1:B:458:ILE:HD12	1:B:473:LEU:HD11	1.94	0.49
1:A:535:LYS:NZ	1:A:568:ARG:O	2.46	0.49
1:B:490:ILE:HG22	1:B:506:GLU:HG2	1.93	0.49
1:B:757:TYR:CZ	1:B:759:HIS:HB2	2.48	0.49
1:B:675:ARG:NH2	1:B:682:GLU:OE1	2.41	0.48
5:D:102:EVP:C15	3:F:9:DT:H1'	2.44	0.48
1:B:1069:PRO:HG2	1:B:1072:GLU:HB3	1.96	0.48
1:A:544:GLN:HB3	1:A:706:PHE:HA	1.96	0.47
3:F:13:DG:H2'	3:F:14:DC:C6	2.50	0.47
1:A:915:ILE:HD11	1:A:985:LEU:HD11	1.96	0.46
1:A:514:VAL:HG21	1:A:536:ILE:HD11	1.98	0.46
1:B:875:ASN:HB3	1:B:1019:LEU:HD21	1.97	0.46
1:A:778:SER:OG	1:A:779:ASN:N	2.48	0.45
1:A:438:ILE:HD11	1:A:512:LYS:HD3	1.98	0.45
1:B:695:TYR:O	1:B:699:ILE:HG12	2.18	0.44
1:B:1148:ARG:HG3	1:B:1149:ASN:N	2.33	0.44
1:A:466:LYS:HD2	1:A:485:PRO:HG3	2.00	0.44
1:A:844:ILE:HD12	1:A:1171:LEU:HD23	2.01	0.43
1:A:951:PRO:HA	1:A:952:PRO:HD3	1.92	0.43
1:B:1085:ASP:HA	1:B:1086:PRO:HD3	1.87	0.43
1:B:757:TYR:CE1	1:B:759:HIS:HB2	2.54	0.43
1:A:675:ARG:NH2	1:A:682:GLU:OE1	2.45	0.43
1:B:597:GLU:OE1	1:B:684:TYR:OH	2.35	0.43
1:B:741:GLU:HB2	1:B:807:PHE:HB3	2.01	0.43
1:A:994:SER:HB3	3:F:20:DT:H5''	2.01	0.42
1:A:495:GLU:HB2	1:A:655:LYS:HD3	2.00	0.42
1:A:719:VAL:HG11	1:A:840:TRP:CE3	2.55	0.42
1:B:764:LEU:HD23	1:B:764:LEU:HA	1.90	0.42
1:B:867:PHE:CZ	1:B:1015:VAL:HG11	2.54	0.42
3:D:13:DG:H2'	3:D:14:DC:C6	2.55	0.42
1:B:916:LEU:HD12	1:B:920:THR:HG22	2.02	0.42
1:A:557:ILE:HG13	1:A:570:LEU:HD11	2.02	0.41
1:A:597:GLU:OE1	1:A:684:TYR:OH	2.28	0.41
1:B:815:ARG:HD2	1:B:820:PRO:HG3	2.01	0.41
1:B:747:LEU:HD23	1:B:768:ILE:HD13	2.02	0.41
1:A:757:TYR:CE1	1:A:759:HIS:HB2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:715:ILE:HA	1:B:716:PRO:HD3	1.82	0.41
1:A:695:TYR:O	1:A:699:ILE:HG12	2.20	0.41
1:B:778:SER:OG	1:B:779:ASN:N	2.48	0.41
1:B:819:PRO:HA	1:B:820:PRO:HD3	1.84	0.41
1:B:670:GLU:HA	1:B:673:ARG:NH1	2.36	0.41
1:A:815:ARG:HD2	1:A:820:PRO:HG3	2.02	0.41
1:A:899:ILE:HG12	1:A:909:ILE:HG12	2.02	0.41
1:B:951:PRO:HA	1:B:952:PRO:HD3	1.89	0.41
1:A:1010:LYS:HD3	1:A:1010:LYS:HA	1.90	0.40
1:B:668:PHE:HB2	1:B:704:ILE:HD11	2.03	0.40
1:B:670:GLU:OE1	1:B:673:ARG:NH1	2.54	0.40
1:A:639:LYS:HD2	1:A:692:TYR:CD2	2.57	0.40
1:B:683:ASP:OD1	1:B:684:TYR:N	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	718/806 (89%)	689 (96%)	29 (4%)	0	100	100
1	B	718/806 (89%)	691 (96%)	27 (4%)	0	100	100
All	All	1436/1612 (89%)	1380 (96%)	56 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	650/724 (90%)	649 (100%)	1 (0%)	93	98
1	B	650/724 (90%)	650 (100%)	0	100	100
All	All	1300/1448 (90%)	1299 (100%)	1 (0%)	93	98

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	913	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	EVP	F	102	-	48,48,48	4.57	24 (50%)	72,73,73	2.73	30 (41%)
5	EVP	D	102	-	48,48,48	4.58	25 (52%)	72,73,73	2.68	28 (38%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EVP	F	102	-	-	2/12/76/76	1/7/7/7
5	EVP	D	102	-	-	2/12/76/76	0/7/7/7

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	102	EVP	C22-C28	-10.37	1.22	1.52
5	F	102	EVP	C22-C28	-10.30	1.22	1.52
5	F	102	EVP	C12-C13	8.95	1.55	1.38
5	D	102	EVP	C12-C13	8.94	1.55	1.38
5	D	102	EVP	C16-C17	8.82	1.52	1.40
5	F	102	EVP	C16-C17	8.72	1.51	1.40
5	F	102	EVP	C18-C17	8.44	1.51	1.40
5	D	102	EVP	C18-C17	8.36	1.51	1.40
5	D	102	EVP	C15-C14	8.28	1.52	1.39
5	F	102	EVP	C19-C14	8.20	1.52	1.39
5	F	102	EVP	C15-C14	8.13	1.51	1.39
5	D	102	EVP	C19-C14	8.13	1.51	1.39
5	F	102	EVP	C3-C2	8.09	1.53	1.38
5	D	102	EVP	C24-C23	-8.02	1.38	1.51
5	D	102	EVP	C3-C2	8.00	1.53	1.38
5	F	102	EVP	C24-C23	-7.73	1.38	1.51
5	F	102	EVP	C4-C5	7.40	1.62	1.51
5	D	102	EVP	C15-C16	7.29	1.52	1.38
5	D	102	EVP	C4-C5	7.23	1.62	1.51
5	F	102	EVP	C19-C18	7.21	1.51	1.38
5	F	102	EVP	C15-C16	7.11	1.51	1.38
5	D	102	EVP	C19-C18	7.07	1.51	1.38
5	F	102	EVP	C3-C4	6.44	1.50	1.39
5	D	102	EVP	C3-C4	6.35	1.50	1.39
5	D	102	EVP	C12-C11	6.04	1.49	1.39
5	F	102	EVP	C12-C11	6.04	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	102	EVP	O3-C7	5.12	1.46	1.35
5	F	102	EVP	O3-C7	5.10	1.46	1.35
5	F	102	EVP	O11-C26	-4.81	1.36	1.44
5	D	102	EVP	O8-C22	4.78	1.55	1.41
5	F	102	EVP	O8-C22	4.74	1.55	1.41
5	D	102	EVP	O11-C26	-4.73	1.36	1.44
5	F	102	EVP	C6-C9	-4.43	1.45	1.54
5	D	102	EVP	C6-C9	-4.41	1.45	1.54
5	D	102	EVP	O9-C22	-3.11	1.34	1.41
5	F	102	EVP	C11-C10	3.07	1.56	1.50
5	D	102	EVP	C11-C10	3.03	1.56	1.50
5	F	102	EVP	O9-C22	-3.01	1.34	1.41
5	F	102	EVP	C6-C5	-3.00	1.50	1.56
5	D	102	EVP	C6-C5	-2.91	1.50	1.56
5	F	102	EVP	O7-C18	2.75	1.41	1.37
5	D	102	EVP	O7-C18	2.66	1.41	1.37
5	D	102	EVP	C14-C5	2.42	1.55	1.52
5	D	102	EVP	O10-C24	-2.32	1.40	1.43
5	D	102	EVP	O2-C1	-2.26	1.39	1.43
5	F	102	EVP	C14-C5	2.26	1.55	1.52
5	F	102	EVP	O2-C1	-2.25	1.39	1.43
5	F	102	EVP	O10-C24	-2.11	1.40	1.43
5	D	102	EVP	C28-C27	-2.02	1.47	1.52

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	102	EVP	O8-C22-O9	-7.33	90.21	110.67
5	D	102	EVP	O11-C26-C27	6.90	122.14	109.75
5	F	102	EVP	O8-C22-O9	-6.88	91.44	110.67
5	F	102	EVP	O11-C26-C27	6.73	121.84	109.75
5	F	102	EVP	O9-C22-C28	6.67	124.46	110.35
5	D	102	EVP	O9-C22-C28	6.56	124.23	110.35
5	F	102	EVP	O5-C16-C17	5.91	120.50	114.54
5	F	102	EVP	C4-C5-C6	5.66	116.11	106.58
5	D	102	EVP	O5-C16-C17	5.53	120.12	114.54
5	D	102	EVP	O7-C18-C17	5.50	120.09	114.54
5	D	102	EVP	C4-C5-C6	5.48	115.79	106.58
5	F	102	EVP	O7-C18-C17	5.36	119.95	114.54
5	F	102	EVP	C27-C26-C23	-5.29	98.80	110.93
5	F	102	EVP	O8-C22-C28	-5.25	94.49	108.10
5	D	102	EVP	O8-C22-C28	-5.04	95.04	108.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	102	EVP	C27-C26-C23	-4.94	99.60	110.93
5	F	102	EVP	O13-C28-C27	-4.91	99.01	110.35
5	D	102	EVP	O13-C28-C27	-4.68	99.52	110.35
5	F	102	EVP	C24-O10-C25	4.54	116.11	111.65
5	D	102	EVP	O3-C7-O4	4.00	125.57	121.42
5	F	102	EVP	O3-C7-O4	3.97	125.54	121.42
5	D	102	EVP	C24-O10-C25	3.71	115.29	111.65
5	D	102	EVP	C22-O8-C10	-3.56	109.21	114.99
5	F	102	EVP	C28-C27-C26	3.39	117.43	109.68
5	D	102	EVP	C8-C9-C6	3.25	106.48	101.79
5	F	102	EVP	O1-C13-C12	3.15	132.07	127.85
5	D	102	EVP	O11-C25-O10	3.15	114.08	110.86
5	F	102	EVP	C22-O8-C10	-3.13	109.90	114.99
5	D	102	EVP	O9-C23-C26	3.10	116.28	109.75
5	D	102	EVP	O1-C13-C12	3.09	131.99	127.85
5	F	102	EVP	C8-C9-C6	3.09	106.25	101.79
5	F	102	EVP	C11-C10-C9	2.97	115.13	111.51
5	F	102	EVP	O2-C2-C3	2.92	131.76	127.85
5	F	102	EVP	O8-C10-C11	2.91	116.04	108.96
5	F	102	EVP	O11-C25-O10	2.90	113.82	110.86
5	D	102	EVP	C28-C27-C26	2.87	116.24	109.68
5	D	102	EVP	O8-C10-C11	2.87	115.93	108.96
5	D	102	EVP	O2-C2-C3	2.83	131.64	127.85
5	D	102	EVP	C11-C10-C9	2.83	114.95	111.51
5	D	102	EVP	C9-C6-C7	2.73	106.72	103.07
5	F	102	EVP	C9-C6-C7	2.72	106.71	103.07
5	F	102	EVP	C8-O3-C7	-2.65	107.86	110.28
5	D	102	EVP	C8-O3-C7	-2.63	107.89	110.28
5	D	102	EVP	O7-C18-C19	-2.61	119.63	124.12
5	F	102	EVP	O4-C7-C6	-2.60	126.03	129.38
5	F	102	EVP	O5-C16-C15	-2.59	119.66	124.12
5	F	102	EVP	O9-C23-C26	2.51	115.05	109.75
5	D	102	EVP	O4-C7-C6	-2.51	126.15	129.38
5	F	102	EVP	O10-C24-C23	2.45	114.37	109.41
5	F	102	EVP	O7-C18-C19	-2.42	119.95	124.12
5	F	102	EVP	O13-C28-C22	-2.37	104.28	110.05
5	F	102	EVP	O3-C8-C9	2.17	107.88	104.71
5	D	102	EVP	O5-C16-C15	-2.17	120.38	124.12
5	D	102	EVP	O13-C28-C22	-2.17	104.77	110.05
5	D	102	EVP	O3-C8-C9	2.16	107.86	104.71
5	D	102	EVP	C20-O5-C16	2.14	120.76	117.53
5	F	102	EVP	O11-C25-C29	2.07	111.13	108.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	102	EVP	C14-C5-C4	-2.06	109.75	112.86

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	F	102	EVP	C17-C16-O5-C20
5	F	102	EVP	C15-C16-O5-C20
5	D	102	EVP	C15-C16-O5-C20
5	D	102	EVP	C17-C16-O5-C20

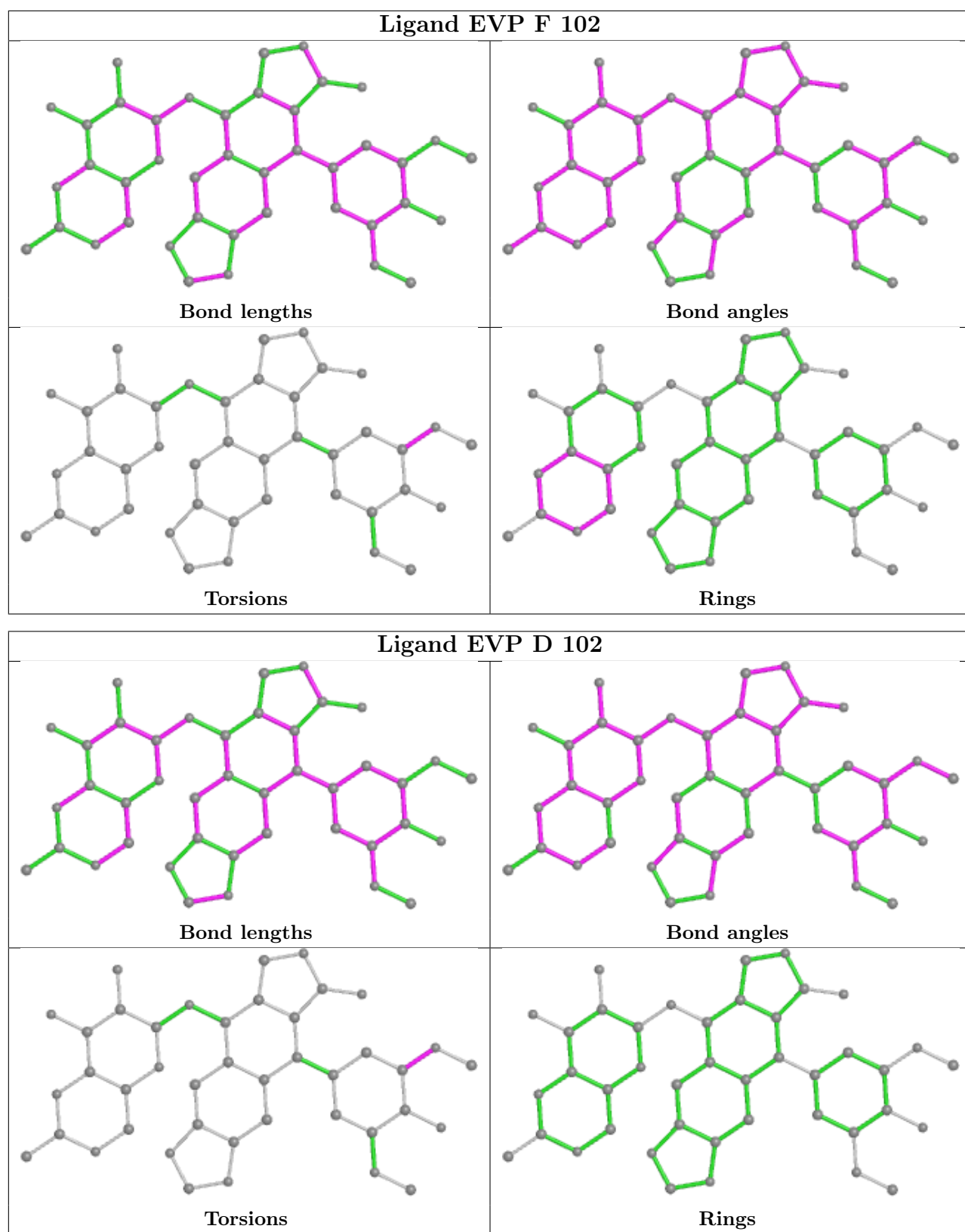
All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	F	102	EVP	C23-C24-C25-C26-O10-O11

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	102	EVP	1	0
5	D	102	EVP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	724/806 (89%)	-0.10	12 (1%) 70 57	54, 100, 154, 209	0
1	B	724/806 (89%)	-0.06	13 (1%) 68 55	56, 107, 168, 191	0
2	C	8/8 (100%)	-0.03	0 100 100	83, 88, 142, 163	0
2	E	8/8 (100%)	0.32	1 (12%) 3 2	79, 97, 145, 182	0
3	D	12/12 (100%)	0.18	1 (8%) 11 6	96, 116, 131, 170	0
3	F	12/12 (100%)	-0.16	0 100 100	93, 112, 124, 147	0
All	All	1488/1652 (90%)	-0.07	27 (1%) 68 55	54, 105, 161, 209	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	475	VAL	6.4
1	A	476	VAL	6.0
1	B	450	ARG	3.7
1	B	474	GLY	3.5
1	A	448	GLY	3.3
2	E	1	DA	3.3
1	A	449	GLY	3.1
1	B	446	ASP	3.1
1	B	475	VAL	3.0
1	B	451	ASN	2.8
1	A	474	GLY	2.8
1	B	476	VAL	2.8
1	A	450	ARG	2.7
1	B	454	GLU	2.6
3	D	20	DT	2.6
1	A	480	LYS	2.5
1	A	451	ASN	2.5
1	A	607	LYS	2.5
1	B	851	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	830	TYR	2.4
1	A	463	ASP	2.3
1	A	477	GLY	2.2
1	B	437	GLY	2.2
1	B	479	ASP	2.2
1	A	550	LYS	2.1
1	B	438	ILE	2.0
1	B	612	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

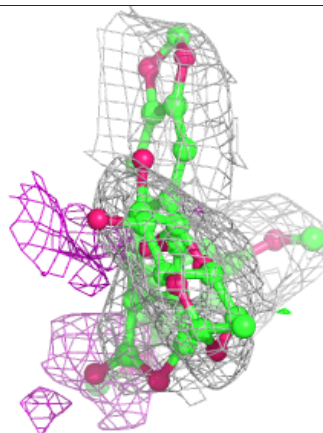
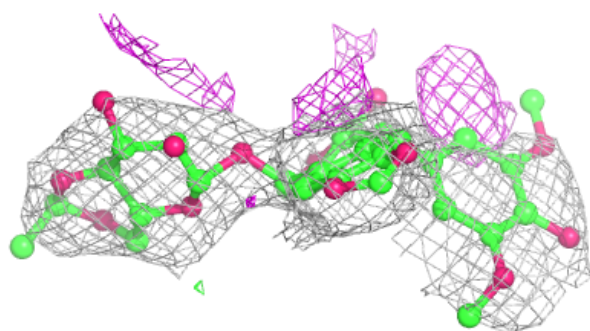
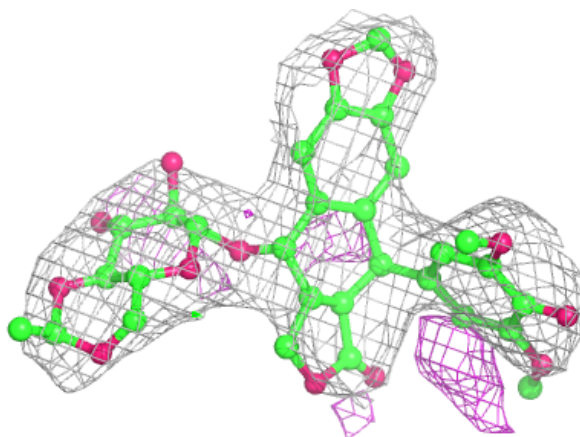
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MG	B	1302	1/1	0.73	1.54	84,84,84,84	0
4	MG	F	101	1/1	0.82	0.63	86,86,86,86	0
4	MG	A	1301	1/1	0.86	0.68	76,76,76,76	0
5	EVP	F	102	42/42	0.89	0.33	82,122,134,136	0
5	EVP	D	102	42/42	0.90	0.29	74,121,130,135	0
4	MG	D	101	1/1	0.90	0.27	80,80,80,80	0
4	MG	B	1301	1/1	0.92	0.66	83,83,83,83	0
4	MG	A	1302	1/1	0.93	1.53	84,84,84,84	0

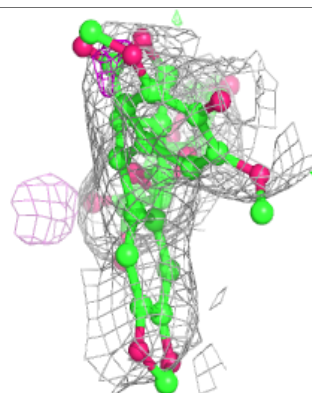
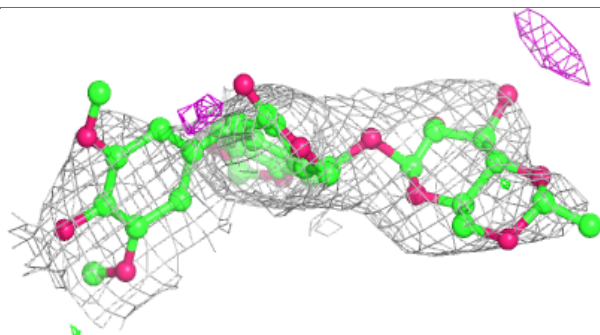
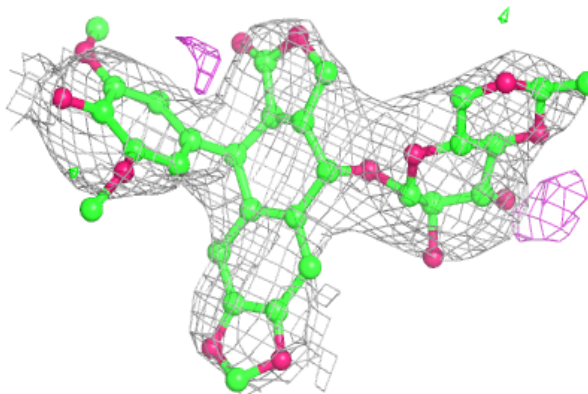
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around EVP F 102:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around EVP D 102:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.